

Electronic spectrum in cuprates within the p-d Hubbard model

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A microscopic theory for electronic spectrum of the CuO₂ plane within an effective *p-d* Hubbard model is proposed. Dyson equation for the one-electron Green function in terms of the Hubbard operators is derived which is solved self-consistently for the self-energy evaluated in the noncrossing approximation. Electron scattering on spin fluctuations induced by kinematical interaction is described by a model dynamical spin susceptibility. Doping and temperature dependence of electron dispersions, spectral functions, the Fermi surface and the coupling constant λ are studied.

Recent ARPES studies revealed a complicated character of electronic structure in the copper oxide superconductors which are believed to be caused by strong electron correlations in cuprates, as was originally suggested by Anderson¹. Below we report the results of electronic spectrum calculations for an effective Hubbard model reduced from the *p-d* model for the CuO₂ plane in cuprates. In these studies for the first time we go beyond the mean-field approximation² or perturbation approach³. We have solved the Dyson equation self-consistently for the thermodynamic Green functions (GFs) and the self-energy derived in the noncrossing approximation (NCA), as has been done by us for the *t-J* model⁴.

I. MODEL AND DYSON EQUATION

We consider an effective *p-d* Hubbard model for one-hole states with energy $\varepsilon_1 = \varepsilon_d - \mu$ and two-hole *p-d* singlet states with energy $\varepsilon_2 = 2\varepsilon_1 + U_{eff}$ where μ is the chemical potential and an effective Coulomb energy $U_{eff} = \Delta_{pd} = \varepsilon_p - \varepsilon_d$ (for details see²):

$$H = \varepsilon_1 \sum_{i,\sigma} X_i^{\sigma\sigma} + \varepsilon_2 \sum_i X_i^{22} + \sum_{i \neq j, \sigma} t_{ij} \{X_i^{\sigma 0} X_j^{0\sigma} + X_i^{\sigma 0} X_j^{0\sigma} + X_i^{2\sigma} X_j^{\sigma 2} + 2\sigma(X_i^{2\bar{\sigma}} X_j^{0\sigma} + \text{H.c.})\}, \quad (1)$$

where $X_i^{nm} = |in\rangle\langle im|$ are the Hubbard operators (HOs) for 4 states $n, m = |0\rangle, |\sigma\rangle, |2\rangle = |\uparrow\downarrow\rangle, \sigma = \pm 1/2, \bar{\sigma} = -\sigma$. The dispersion of holes is determined by the hopping parameters: $t_{ij} = t\delta_{j,i \pm a_{x/y}} + t'\delta_{j,i \pm a_x \pm a_y}$ ($a_{x/y} = a$ - lattice constants). We take $\Delta_{pd} = 8t \simeq 3.2$ eV and $t' = -0.3t < 0$.

By applying the Mori-type projection technique for the GFs $G_{ij\sigma}(t-t') = \langle\langle \hat{X}_{i\sigma}(t) | \hat{X}_{j\sigma}^\dagger(t') \rangle\rangle$ in terms of the two-component HOs ($\hat{X}_{i\sigma}^\dagger = \{X_i^{2\sigma}, X_i^{\sigma 0}\}$) an exact Dyson equation was derived as described in² with a self-energy (SE) as a many-particle GF. By using NCA for the SE, a closed system of equations was obtained for the the GFs and the SE:

$$\tilde{G}_{1(2)}(\mathbf{q}, \omega) = (\omega - \tilde{\varepsilon}_{1(2)}(\mathbf{q}) - \tilde{\Sigma}(\mathbf{q}, \omega))^{-1}, \quad (2)$$

where $\tilde{\varepsilon}_{1(2)}(\mathbf{q})$ are spectra for two bands given by the matrix $\tilde{\varepsilon}_{ij} = \langle\langle [\hat{X}_{i\sigma}, H], \hat{X}_{j\sigma}^\dagger \rangle\rangle \times \langle\langle \hat{X}_{i\sigma}, \hat{X}_{i\sigma}^\dagger \rangle\rangle^{-1}$. The SE is the same for the both Hubbard bands:

$$\tilde{\Sigma}(\mathbf{k}, \omega) = \frac{1}{\pi^2 N} \sum_{\mathbf{q}} |t(\mathbf{q})|^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\nu dz N(z, \nu)}{\omega - z - \nu} \times \text{Im} \chi_{sc}(\mathbf{k} - \mathbf{q}, \nu) \text{Im} \{\tilde{G}_1(\mathbf{q}, z) + \tilde{G}_2(\mathbf{q}, z)\}. \quad (3)$$

Here the interaction $t(\mathbf{q})$ is determined by the hopping parameter t_{ij} , $N(z, \nu) = (1/2)(\tanh(z/2T) + \coth(\nu/2T))$ and $\chi_{sc}(\mathbf{q}, \nu) = \frac{1}{4} \langle\langle N_{\mathbf{q}} | N_{-\mathbf{q}} \rangle\rangle_{\nu} + \langle\langle \mathbf{S}_{\mathbf{q}} | \mathbf{S}_{-\mathbf{q}} \rangle\rangle_{\nu}$ is the charge-spin susceptibility where $N_{\mathbf{q}}$ is the number and $\mathbf{S}_{\mathbf{q}}$ is the spin operators.

II. RESULTS AND DISCUSSIONS

The system of equations (2), (3) was solved numerically for various hole concentrations $n = 1 + \delta = 2\langle X_i^{\sigma\sigma} + X_i^{22} \rangle$ by using the Matsubara frequency representation at temperature $T \simeq 0.03t \simeq 140$ K. Neglecting charge fluctuations, the spin susceptibility was described by the model: $\text{Im} \chi_s(\mathbf{q}, \nu) = \chi_0 / [1 + \xi^2(1 + \gamma(\mathbf{q})) \tanh(\nu/2T) / [1 + (\nu/\omega_s)^2]]$ where ξ is an antiferromagnetic (AF) correlation length (in units of a), $\omega_s \simeq J = 0.4t$ is spin-fluctuation energy, and $\gamma(\mathbf{q}) = (1/2)(\cos q_x + \cos q_y)$. The constant $\chi_0 = [3(1 - |\delta|)/2\omega_s] \{ (1/N) \sum_{\mathbf{q}} [1 + \xi^2(1 + \gamma(\mathbf{q}))]^{-1} \}^{-1}$ is defined from the equation $\langle \mathbf{S}_i \mathbf{S}_i \rangle = (3/4)(1 - |\delta|)$.

The dispersion curves given by maxima of spectral functions $A(\mathbf{k}, \omega) = B_1(\mathbf{k}) \hat{A}_1(\mathbf{k}, \omega) + B_2(\mathbf{k}) \hat{A}_2(\mathbf{k}, \omega)$, where $B_{1,2}(\mathbf{k})$ are the weights of the bands and $\hat{A}_{1(2)}(\mathbf{k}, \omega) = -(1/\pi) \text{Im} \tilde{G}_{1(2)}(\mathbf{k}, \omega)$, were calculated for hole doping $\delta = 0.1 - 0.3$. The dispersion curves and the spectral function for $\delta = 0.1$ ($\xi = 2.5$) reveal a rather flat hole-doped band at the Fermi energy (FE) ($\omega = 0$) (Fig. 1, Fig. 2).

At high temperature $T = 0.3t$ for $\delta = 0.1$ ($\xi = 1.0$) (Fig. 3, Fig. 4) or in the overdoped region ($\delta = 0.3$) the dispersion becomes much larger which proves a strong influence of AF spin-fluctuations on the

With doping, the density of states (DOS) shows a weight transfer from the upper to the lower band as

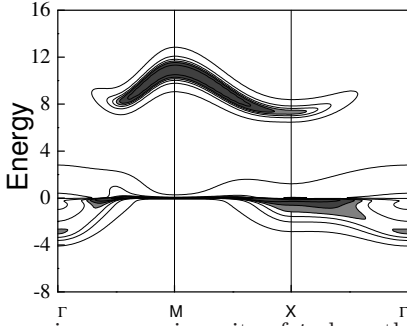


FIG. 1: Dispersion curves in units of t along the symmetry directions $\Gamma(0,0) \rightarrow M(\pi,\pi) \rightarrow X(\pi,0) \rightarrow \Gamma(0,0)$ for $\delta = 0.1$ and temperature $T = 0.03t$.

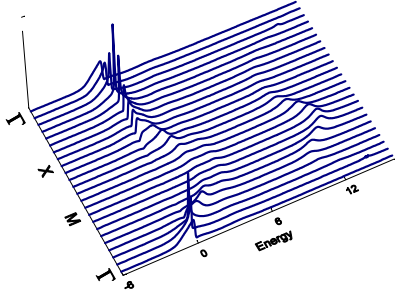


FIG. 2: Spectral function in units of t along the symmetry directions $\Gamma(0,0) \rightarrow M(\pi,\pi) \rightarrow X(\pi,0) \rightarrow \Gamma(0,0)$ for $\delta = 0.1$ and temperature $T = 0.03t$.

shown in Fig. 5, left panel. The self-energy $\tilde{\Sigma}(\mathbf{k},\omega)$ reveals an appreciable variation with \mathbf{k} and doping close to the Fermi level. Figure 6 shows a change of dispersion (kink) in the $M \rightarrow X$ direction at the Fermi level crossing for $\delta = 0.1$. For the coupling constant we get an estimation $\lambda = v_F/v_0 - 1 \simeq 2.4$ ($\lambda \simeq 0.7$ for $\delta = 0.3$).

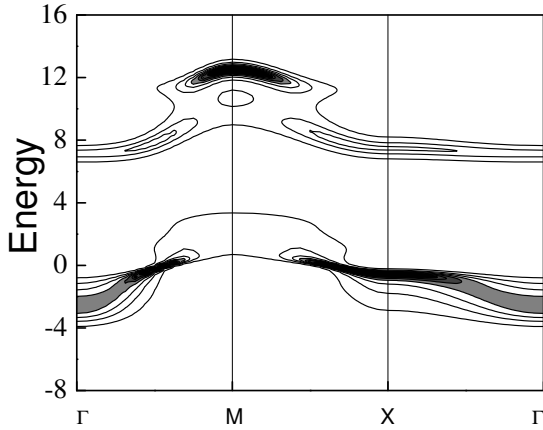


FIG. 3: The same as Fig. 1 but for $T = 0.3t$.

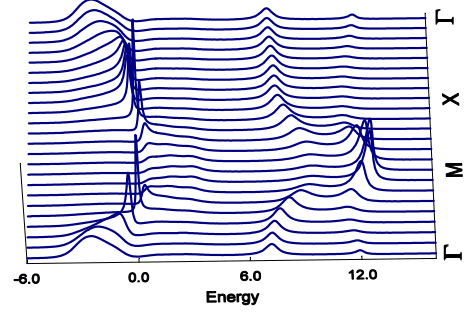


FIG. 4: The same as Fig. 2 but for $T = 0.3t$.

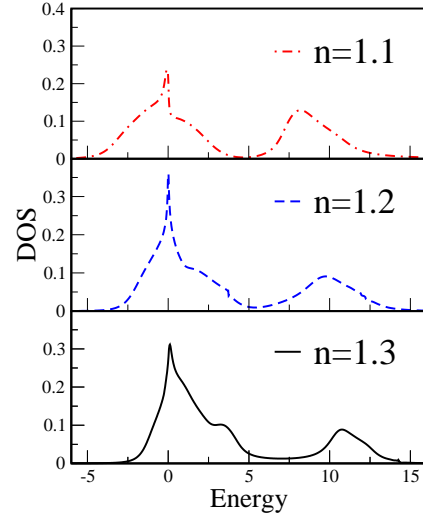


FIG. 5: Electronic density of states.

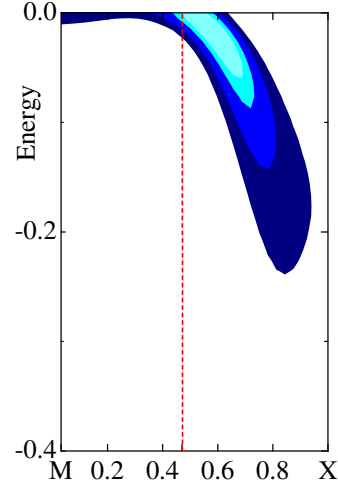


FIG. 6: $A(\mathbf{k},\omega)$ in the $M \rightarrow X$ direction at the Fermi level crossing for $\delta = 0.1$.

The FS changes from a hole arc-type at $\delta = 0.1$ to an electron-like one at $\delta = 0.3$ (Fig. 7 – Fig. 9).

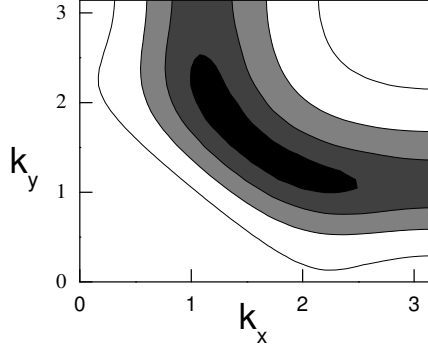


FIG. 7: $A(\mathbf{k}, \omega = 0)$ on the FS for $\delta = 0.1$.

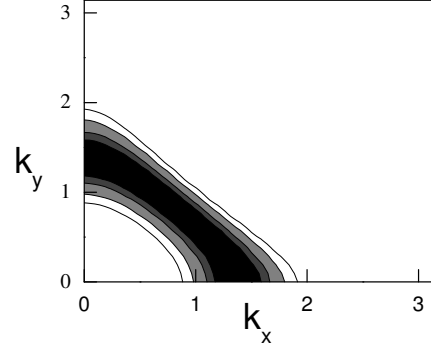


FIG. 9: The same as Fig. 7 but for $\delta = 0.3$.

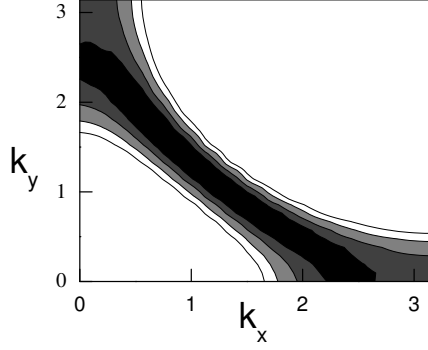


FIG. 8: The same as Fig. 7 but for $\delta = 0.2$.

To conclude, the microscopic theory based on HO technique for the effective p - d model (1) provides an explanation for doping and temperature dependence of electronic spectrum in cuprates which is controlled by the AF spin correlations. Superconducting pairing in the model beyond the weak coupling approximation⁵ will be considered elsewhere.

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